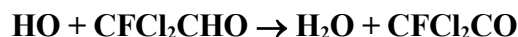


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.142 oClOx68

Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

This datasheet last evaluated: June 2015; last change in preferred values: December 2003.



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.3 \pm 0.1) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	PLP-RF
<i>Relative Rate Coefficients</i>			
$(1.0 \pm 0.2) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of CH_3ONO or $\text{C}_2\text{H}_5\text{ONO}$ in CH_3ONO (or $\text{C}_2\text{H}_5\text{ONO}$)- CFCl_2CHO -toluene-air mixtures at 987 ± 13 mbar pressure. The concentrations of CFCl_2CHO and toluene were measured by GC and/or FTIR spectroscopy. The measured rate coefficient ratio of $k(\text{HO} + \text{CFCl}_2\text{CHO})/k(\text{HO} + \text{toluene}) = 0.184 \pm 0.034$ is placed on an absolute basis using $k(\text{HO} + \text{toluene}) = 5.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Calvert et al., 2002). Scollard et al. (1993) did not report a value for the rate coefficient ratio $k(\text{HO} + \text{CFCl}_2\text{CHO})/k(\text{HO} + \text{toluene})$. Dividing the reported value of $k(\text{HO} + \text{CFCl}_2\text{CHO})$ by the value of $k(\text{HO} + \text{toluene})$ used by Scollard et al. (1993) gives $k(\text{HO} + \text{CFCl}_2\text{CHO})/k(\text{HO} + \text{toluene}) = 0.184 \pm 0.034$ which is placed on an absolute basis in the table above using a rate coefficient of $k(\text{HO} + \text{toluene}) = 5.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Calvert et al., 2002).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.2×10^{-12}	298
<i>Reliability</i>		
$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The preferred value is an average of the absolute and relative rate coefficients of Scollard et al. (1993), which are in good agreement.

References

Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J. and Yarwood, G.: The Mechanism of Atmospheric Oxidation of Aromatic Hydrocarbons,

Oxford University Press, New York, NY, 2002.

Scollard, D. J., Treacy, J. J., Sidebottom, H. W., Balestra-Garcia, C., Laverdet, G., LeBras, G., MacLeod, H. and Téton, S.: *J. Phys. Chem.*, 97, 4683, 1993.